Ion Mobility Analysis of Gaseous and Particulate Pollutants

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The Ideal Aerosol Chemical Analysis Instrument

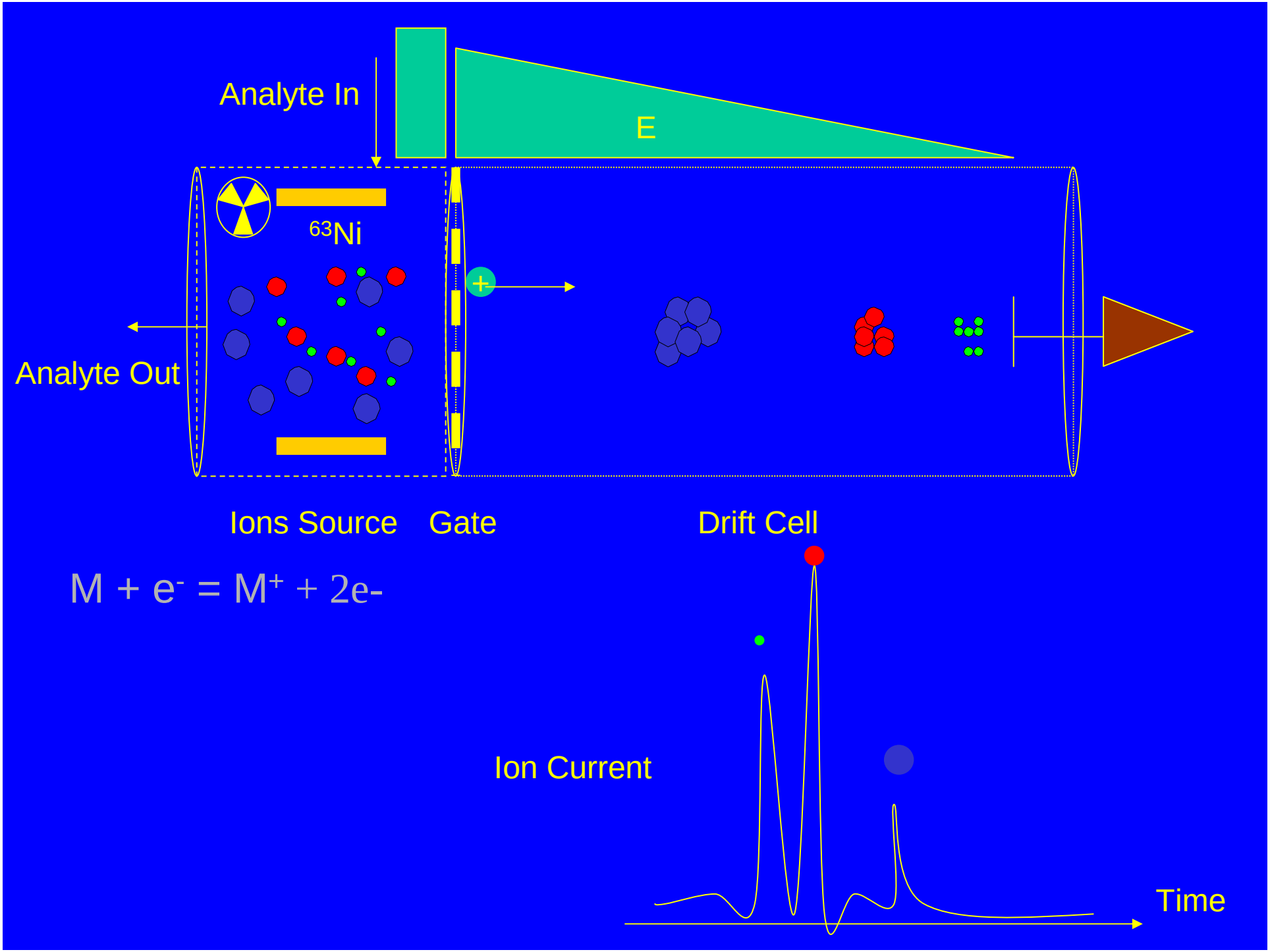
- Goals
  - High Time Resolution
  - Inexpensive capital and operating costs
    - Nice goal in its own right
    - Allows high spatial resolution
  - Chemical Speciation
    - Goes along with cheap – obviates the need for multiple toys
    - Nail those organics
- Instrument Characteristics
  - Fast = real time, spectrometry
  - Cheap = No Vacuum
  - Chemical Analysis = a separation technology

A separation technology: Ion electrical mobility

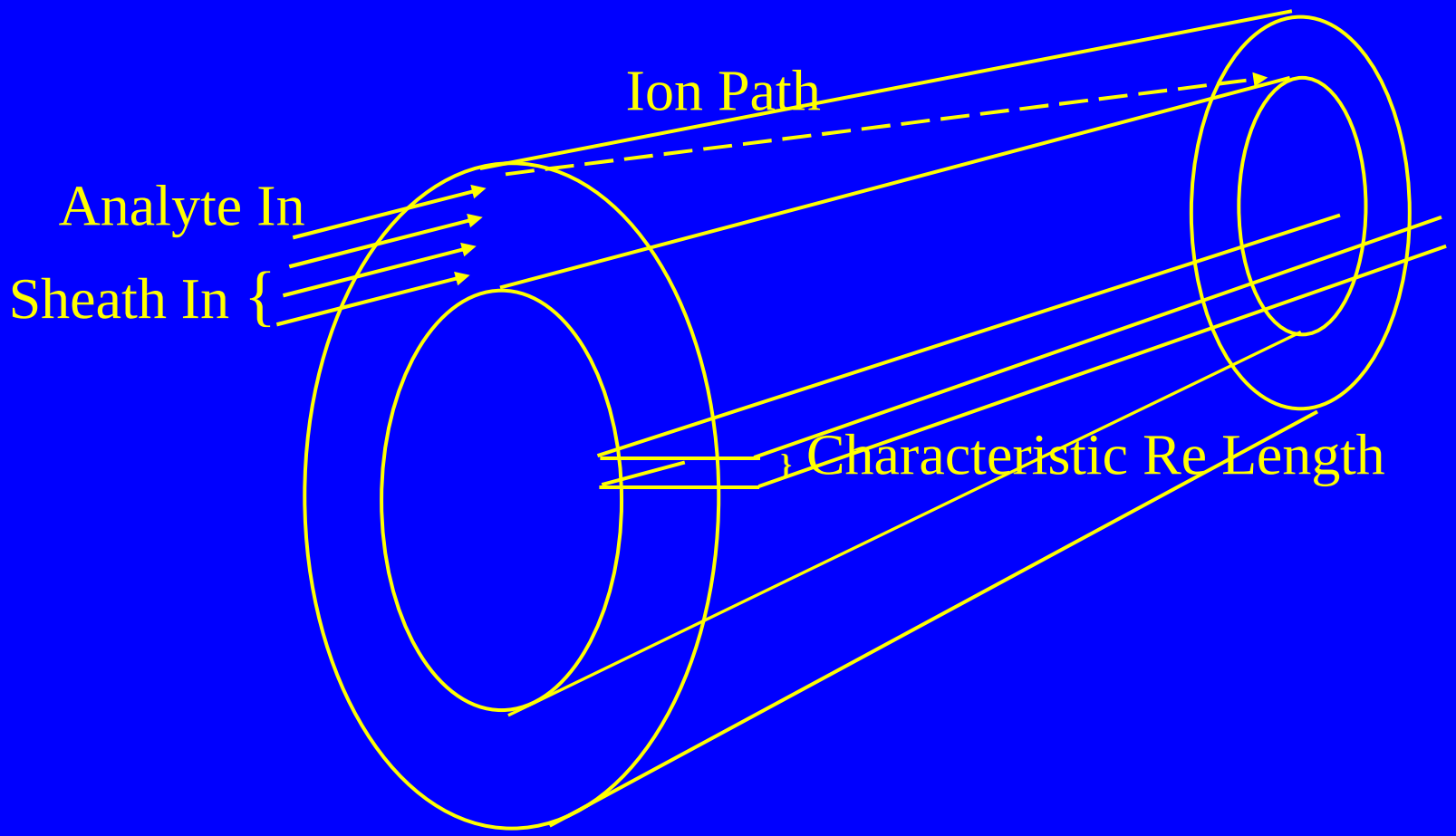
- V_{drift}=ZE is the drift velocity [cm/s]
- Z is electric mobility [cm/s]/[volt/cm]
- E is electric field strength [volt/cm]
- Einstein Relation between mobility and diffusivity, D, limits resolution
  - D=kTZ/q
  - q is charge – usually +/-1 for molecular ions
- Z is function of ion or particle size, charge, E!
  - Ion mobility range: 0.5-3.0
  - Particle mobility range: 10^{-2}-10^{-5}

Ion Mobility Spectrometry

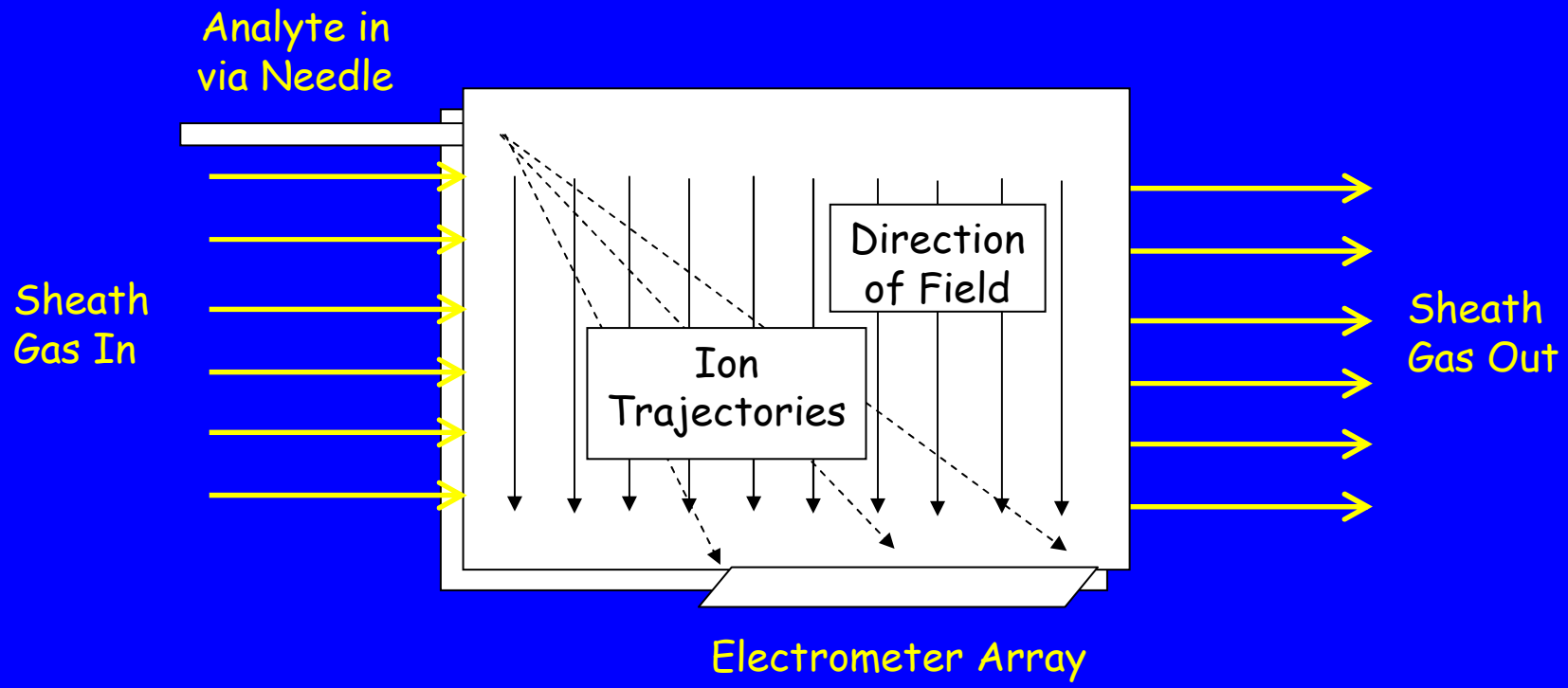
- Time-of-Flight (temporal separation)
  - Used and studied for decades
    - See Eiceman and Karpas, second edition
    - Inexpensive, fast, ion mobility separation
  - Currently used in airports, by the military
    - Detection of explosive, toxins, etc.
  - Limited application in the atmosphere, so far
    - Resolution – sensitivity trade-offs
    - Water/temperature/analyte interference
    - Not very quantitative



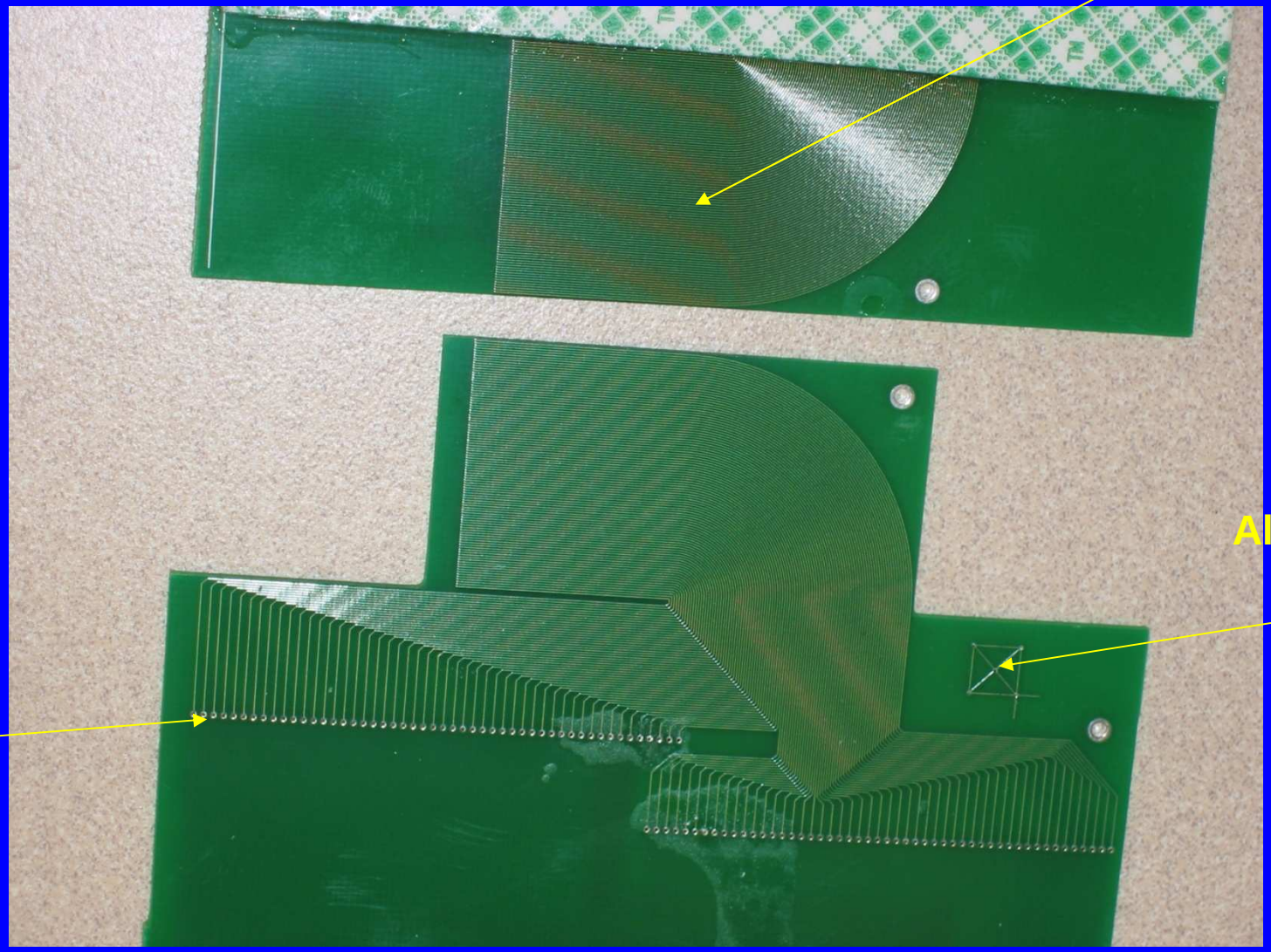
DMA Technology



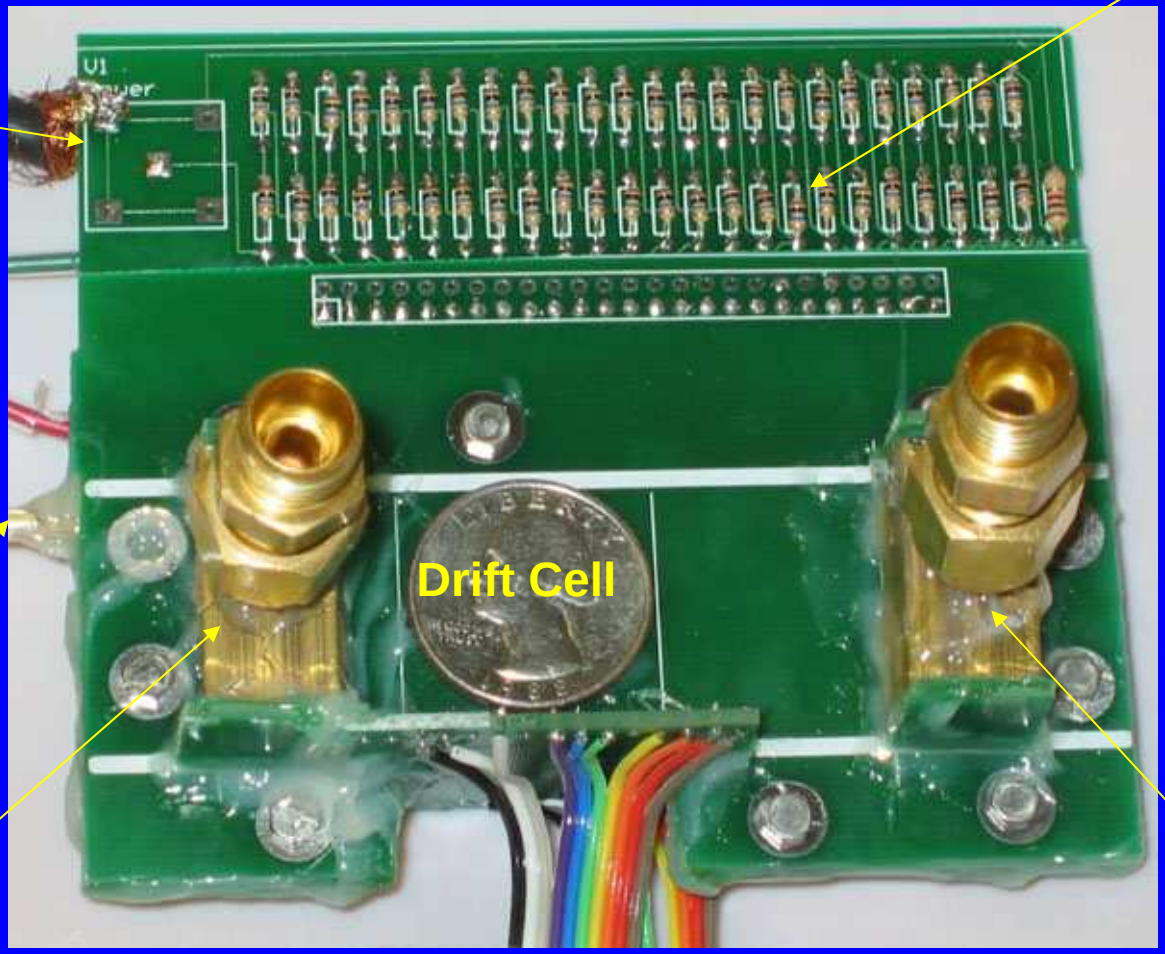
Cross Flow - Ion Mobility Spectrometry
CF-IMS Schematic



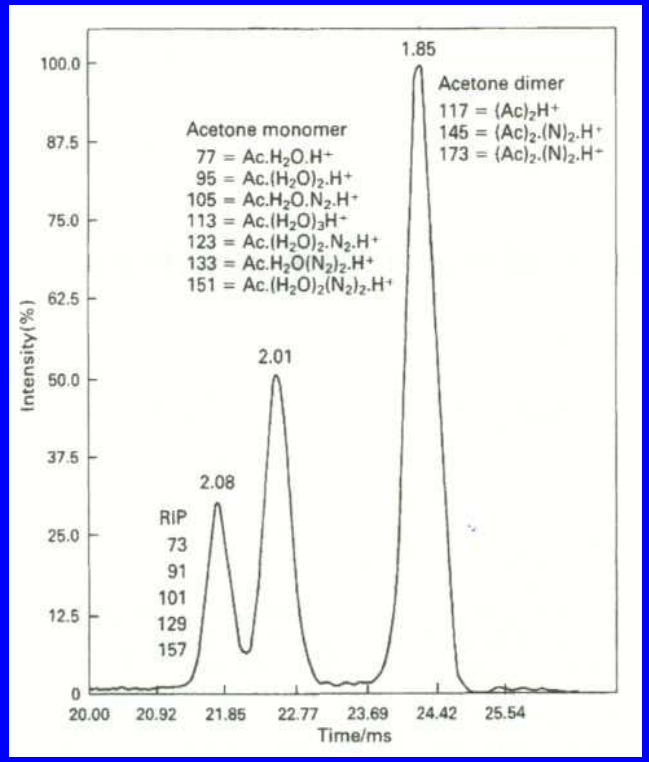
Drift Cell Open Showing Traces

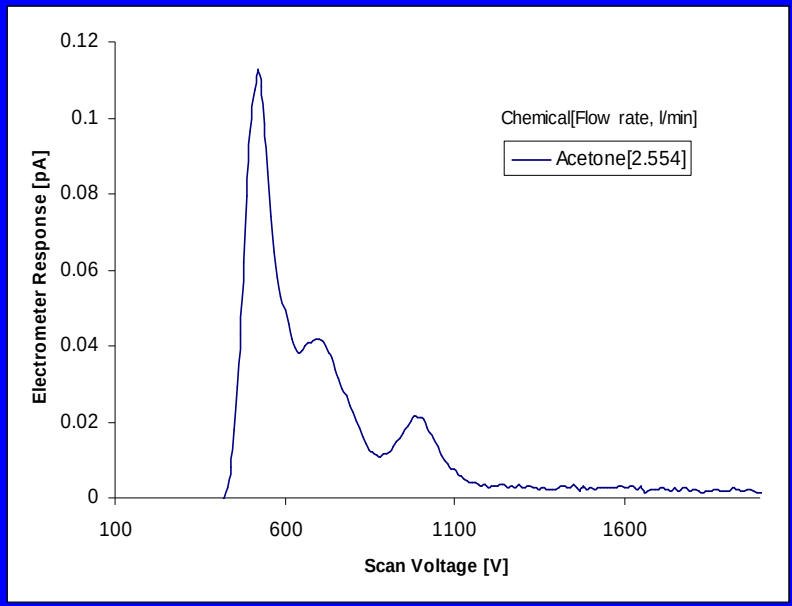


Low Resolution Prototype



Acetone Ion Mobility Spectrum





Zhang, M. and A.S. Wexler. Cross Flow Ion Mobility Spectrometry: Theory and Initial Prototype Testing. *Int´l J. Mass Spectrometry* 258:13-20, 2006.

CF-IMS

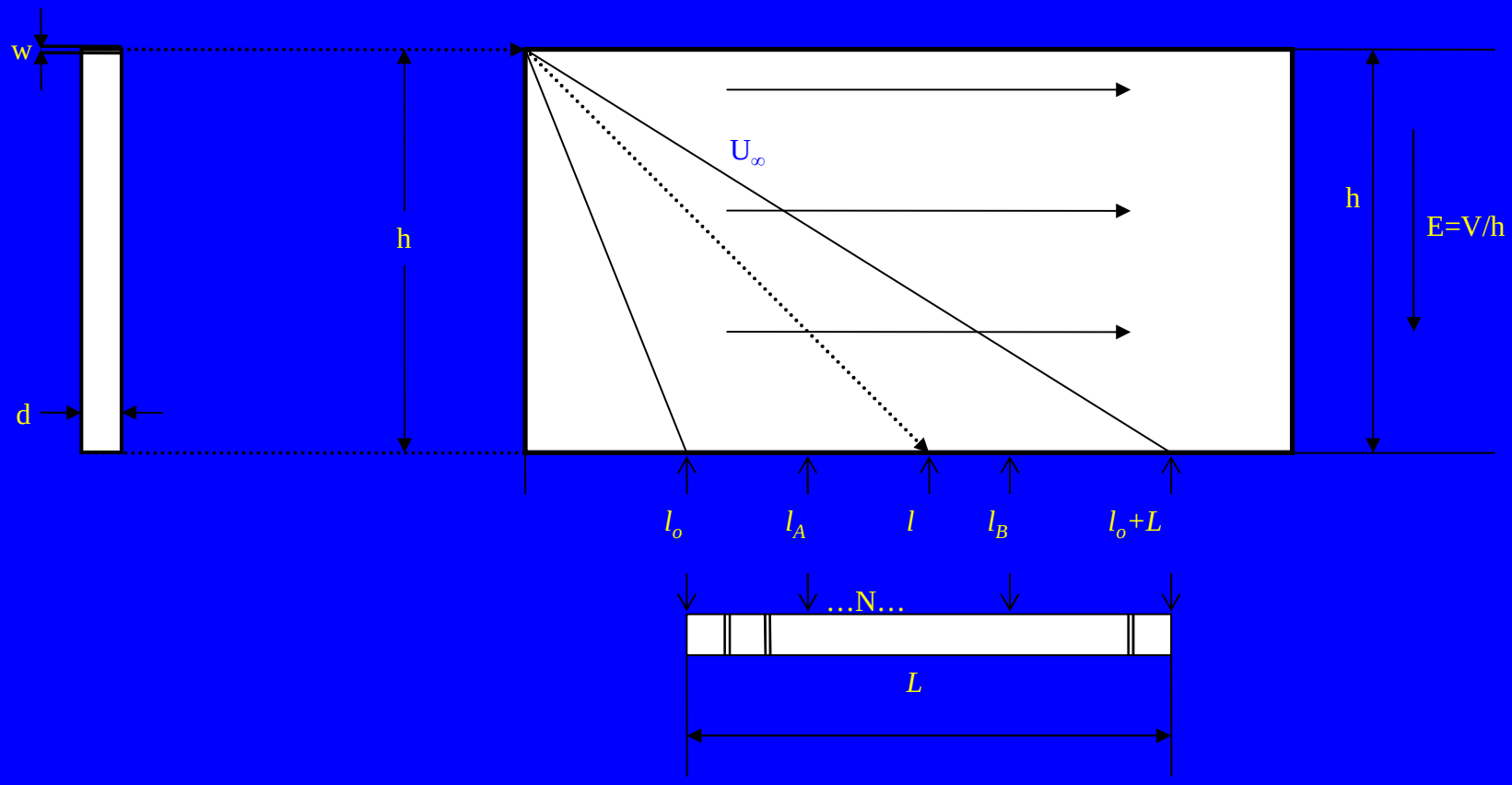
- What's Next?
  - High Resolution
  - Electrometer Array
  - Gas and Particle Analysis
  - Manufacturability

CF-IMS Resolution

- Resolution Challenges
  - Diffusion
  - Geometric Aberration
  - Parabolic Flow Profile
- Resolution-Sensitivity Trade-offs
  - Needle Width and Height
  - Electrometer Pad Size
- Sensitivity Challenges
  - Electrometer Fantastic-ness

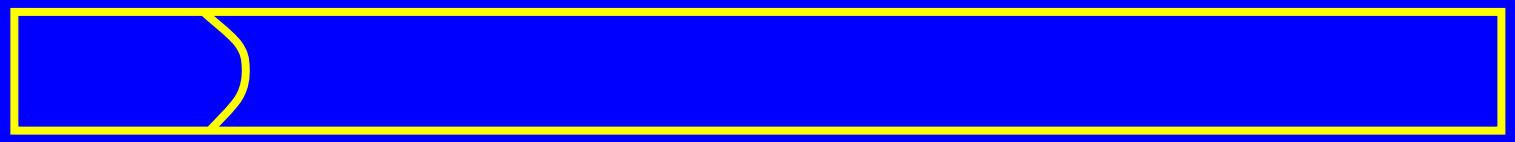
CF-IMS Resolution: Needle width and diffusion

$$R^{-1} = \frac{w}{h} + \frac{\Delta l}{l} + \frac{2\delta_x \sqrt{h^2 + l^2}}{hl}$$



CF-IMS Resolution: Dispersion in the Gap

- Flow in gap is parabolic
- Center faster than periphery dispersing ions
  - Center ions reach their electrode at $l(0)$
  - Ions x from center: $l(x) = l(0)[1-(x / d/2)^2]$
- Resolution, R^{-1}, is
  - $R^{-1} = \{l(0) - l(x)\}/l(0) = (x / d/2)^2$



CF-IMS Design Criteria

- Flow in gap is laminar
- Field gradient less than break down voltage
- Same needle and sheath gas velocities
  - Minimize eddies
- Balance Sources of Resolution Loss
  - Dispersion
  - Diffusion
  - Needle size
    - Geometric aberration
    - Flow dispersion
  - Electrometer pad size

CF-IMS Low and High Resolution Specifications

Prototypes	High Resolution	Low Resolution
Dimension L×W×H[cm]	20×10×0.1	2.5×2.5×0.16
Sample Flow Rate [cc/s]	4.2	5
Sheath Gas Flow Rate [l/min]	110	3-5
Recirculation Blower Power [W]	0.8	N/A
Mobility Range [cm^2/v-s]	1.5-3.0	1.0-2.5
Molar Mass Range	30-600 Dalton	30-600 Dalton
Sample Flow Pressure Drop [Pa]	64	<1
Sheath Flow Pressure Drop [Pa]	435	<1
Power Supply Voltage (kV)	10	5
Sensor Length [cm]	10	2.54
Electrometer Pad Size L×d [cm×cm]	0.02×0.1	0.08×0.16
Mobility Resolution	92	10

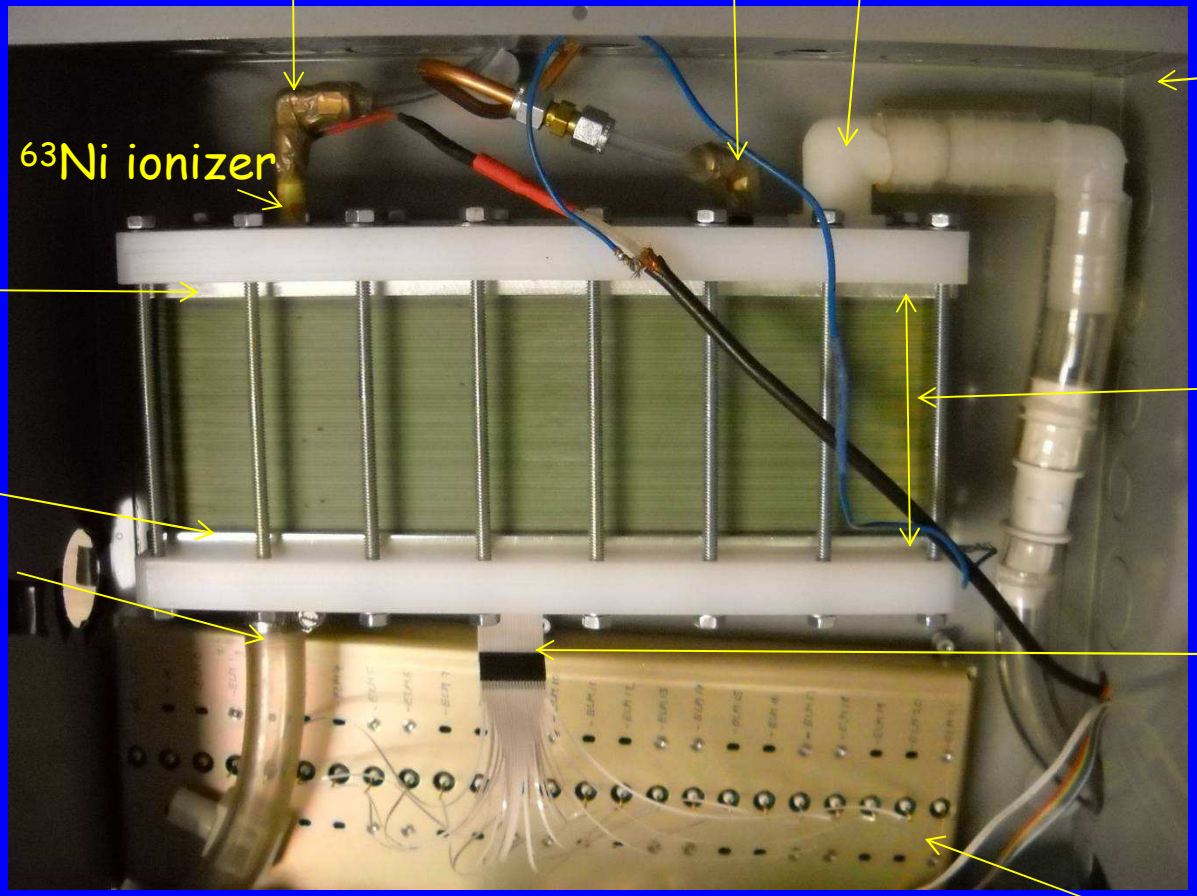
CF-IMS Electrometer Array

Perkin Elmer XL-1256

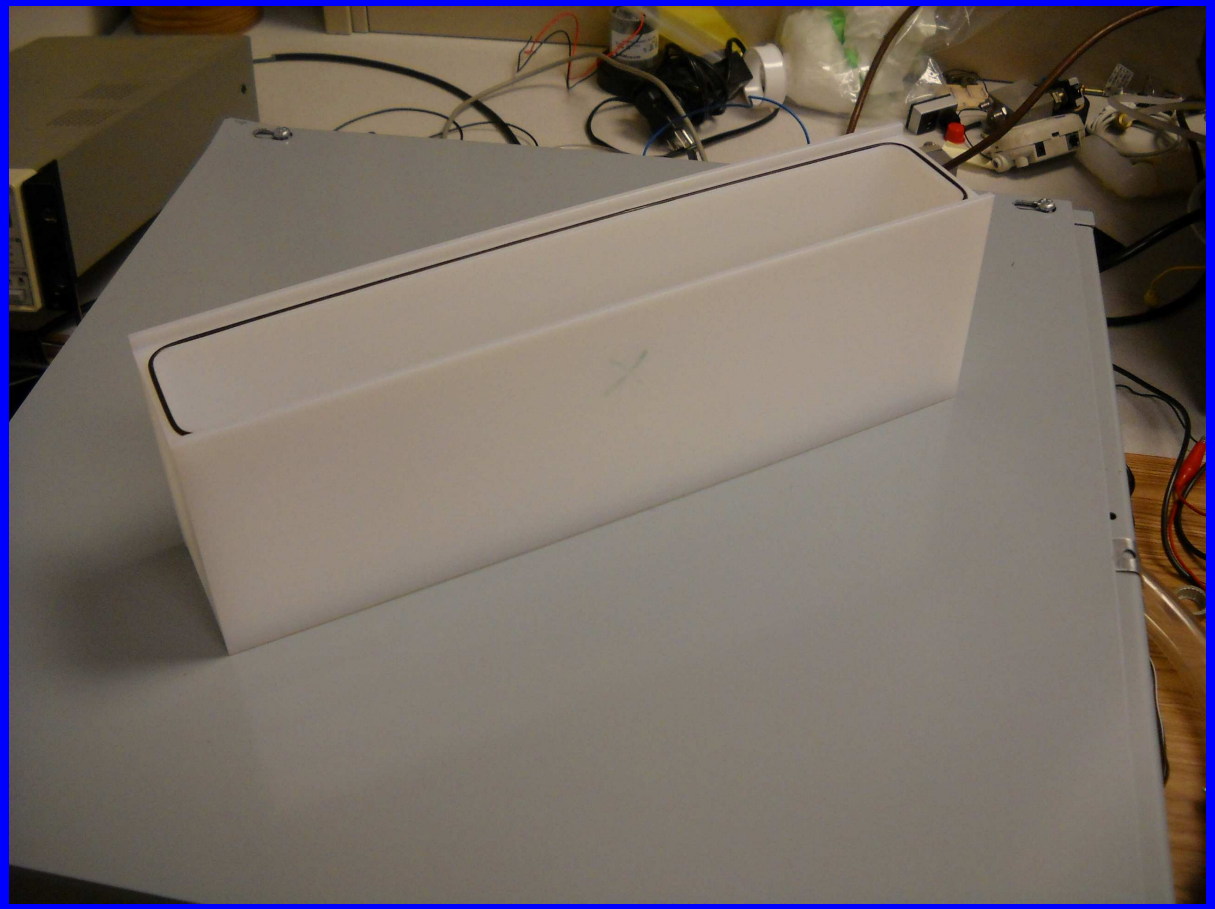
Table 2. Specifications

Description	Min	Nom	Max	Units
Saturation charge	2.5[5]		40.5[6]	pC
Parasitic input capacitance (to V_{SS})		4.5		pF
Input leakage current (per channel)		±100	±250	fA
Charge conversion	10^6		160[5]	nV/e-
Integration amplifier slew rate		1.0		V/µsec
Output clocked video level (V_{REF}=5V)				
Q: 0 to QSAT	3.0	2.5	1.5	V
Q: 0 to -QSAT	6.5	7.5	8.5	V
Output quiescent video level		V_{REF}		V
Output video impedance		1.5		K ohm
Output video readout frequency			1.0	MHz
VoutS output variation[1]		15		mV
VoutR output variation[1]		15		mV
Video output differential offset[2]		40		mV
Digital outputs (EOL signal) high level	3.5		5.5	V
Digital outputs (EOL signal) low level	GND		GND+0.3	V
Quiescent V_{DD} current (I_{DD})		40	45	mA
Clocked V_{DD} current		50	55	mA
PSRR (@1kHz & 120 pF C_{IN}) To V_{SS}			-25	dB
PSRR (@1kHz & 120 pF C_{IN}) To V_{DD}			-25	dB
Operating potential (V_{DD}–V_{SS})	9.5	10	12.5	V
Reference potential		5	7	V
Digital input levels–high level	3.5	5	5	V
Digital Input levels–low level	GND	GND	0.4	V
Bias resistor current		16		µA
Operating temperature range	0		70	°C
Noise @25 pFC_{IN}[3]				
Input referred noise		5		µVms
		29		rms electrons
System noise		70		µVms
		450		rms electrons
Dynamic range[4]	90			dB

CF-IMS High Resolution Prototype



CF-IMS High Resolution Prototype Components



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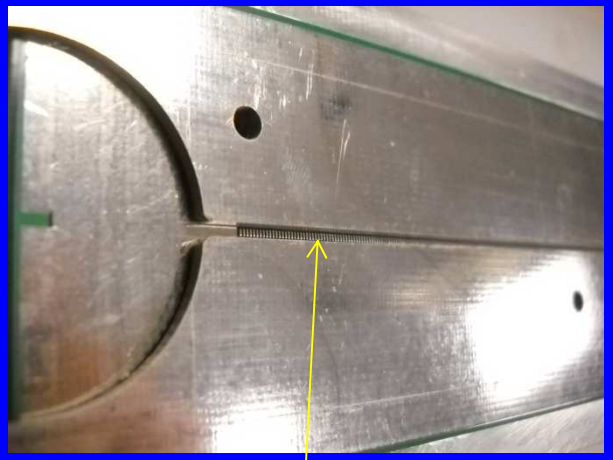
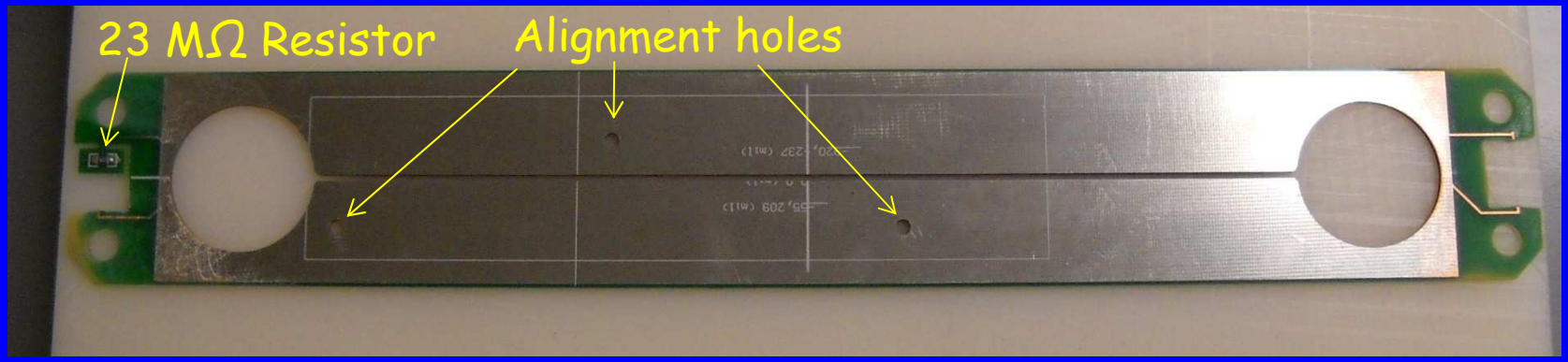


Electrometer pads



PCB Board

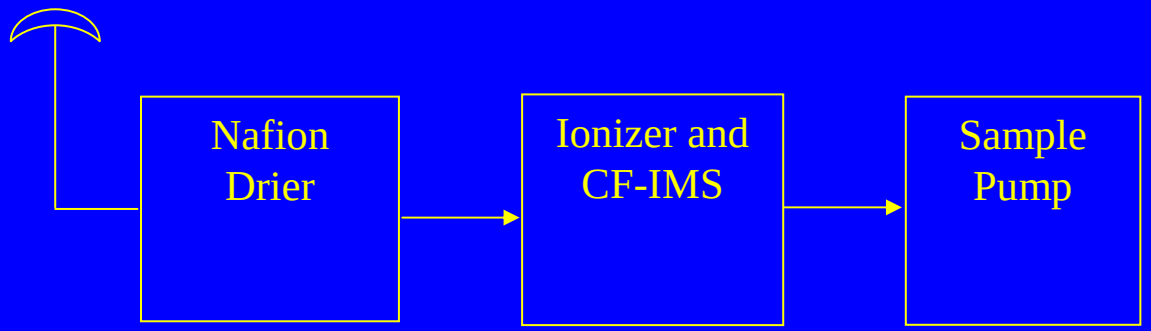
Manufacturability

- ↑ High Voltage / Automatic Voltage Divider
- ↑ E-field parallel to flow channel
- ↓ Leaks – Sleeve fixes that

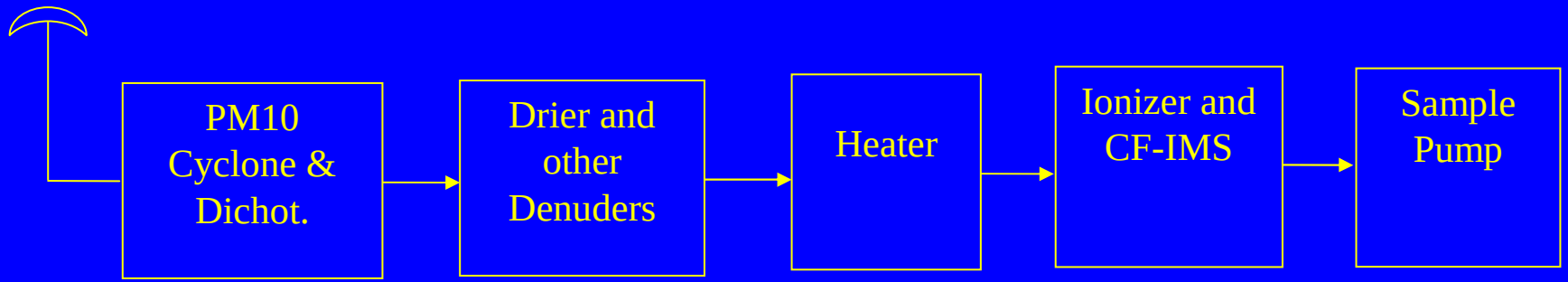
Current (literally) Issues

- Leaks
  - Seem to have leaks between the boards fixed
  - Seem to have blower leaks fixed too
- Current
  - 10 mCi should produce ~20-30 nA current
  - Diffusion losses take this to ~7-10 nA
  - Actual is about 1 pA (10^4 loss)
  - Measurement and SIMION calcs show low loss in IMS cell
  - When we find loss, pad current will be ~40 pA

CF-IMS – Instrument Realizations



Schematic for analysis of gas phase precursors



Schematic for analysis of semi-volatile particulate compounds

How much might it cost?

- Electrometer arrays 2@$300=$600
- Electrometer-PC interface $400
- Pumps $200
- PC boards $200
- Endcaps $100
- 6" ruler $1
- Total parts cost $1501
- Manufacturer's markup $6000
- Total list price $7501
- Double for particle conditioning add-ons

Thank You

- Mang Zhang and Sonya Collier
  - For doing all the work
- Dreyfus Foundation, CARB and EPA
  - For supporting this work
- You
  - For staying awake
- Questions?